



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2021 – 09:04 PM EDT

PDB ID : 1RIF  
Title : Crystal structure of the UvsW helicase from Bacteriophage T4  
Authors : Sickmier, E.A.; White, S.W.; Kreuzer, K.N.  
Deposited on : 2003-11-17  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

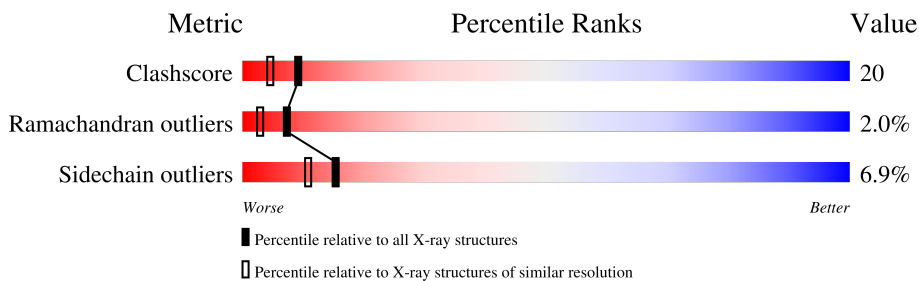
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	282	 64% 30% 6%
1	B	282	 67% 29% .

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4891 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA helicase uvsW.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	282	2315	1489	397	416	13	0	0	0
1	B	282	2315	1489	397	416	13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	ARG	LYS	engineered mutation	UNP P20703
B	141	ARG	LYS	engineered mutation	UNP P20703

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0
2	B	2	2	2	0	0

- Molecule 3 is GOLD ION (three-letter code: AU) (formula: Au).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Au		
3	A	2	2	2	0	0
3	B	2	2	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	132	132	132	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	B	122	Total 122	O 122	0	0

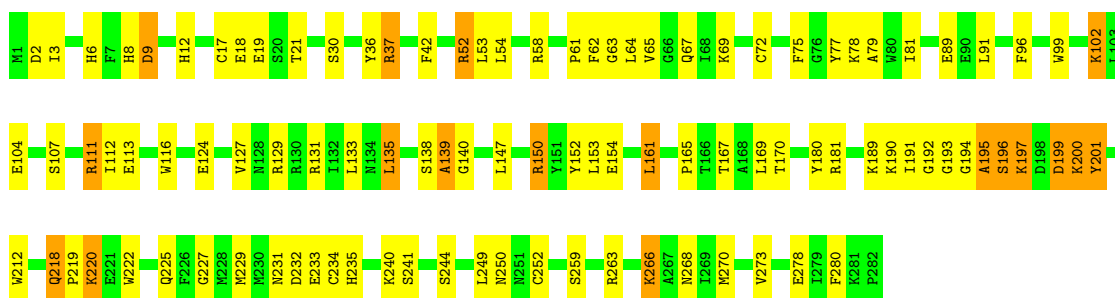
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

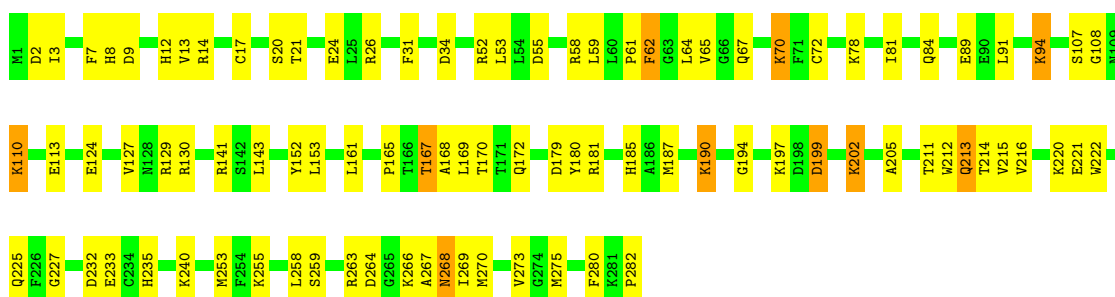
- Molecule 1: DNA helicase uvsW

Chain A:  64% 30% 6%



- Molecule 1: DNA helicase uvsW

Chain B:  67% 29% 4%



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.74Å 95.18Å 86.28Å 90.00° 95.40° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.00)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.218 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4891	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.39	0/2375	0.64	0/3195
1	B	0.39	0/2375	0.64	0/3195
All	All	0.39	0/4750	0.64	0/6390

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2315	0	2265	106	0
1	B	2315	0	2265	79	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	132	0	0	8	0
4	B	122	0	0	15	0
All	All	4891	0	4530	183	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (183) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LYS:HA	1:A:78:LYS:HE2	1.54	0.87
1:A:111:ARG:HB3	1:A:111:ARG:HH11	1.39	0.87
1:B:94:LYS:HD3	1:B:94:LYS:H	1.40	0.85
1:A:91:LEU:HD11	1:A:96:PHE:HB2	1.57	0.85
1:A:112:ILE:HB	4:A:407:HOH:O	1.78	0.84
1:A:190:LYS:HB2	1:A:196:SER:H	1.47	0.80
1:B:124:GLU:HG2	4:B:336:HOH:O	1.82	0.79
1:B:214:THR:HG21	4:B:303:HOH:O	1.83	0.78
1:A:111:ARG:HH11	1:A:111:ARG:CB	1.99	0.76
1:B:211:THR:OG1	1:B:213:GLN:HG3	1.84	0.76
1:B:89:GLU:HB2	1:B:127:VAL:HA	1.68	0.74
1:B:61:PRO:HG2	1:B:64:LEU:HD12	1.69	0.74
1:B:94:LYS:H	1:B:94:LYS:CD	2.00	0.74
1:A:196:SER:HB2	1:A:200:LYS:HG3	1.69	0.73
1:A:91:LEU:CD1	1:A:96:PHE:HB2	2.18	0.73
1:A:263:ARG:HE	1:A:266:LYS:HG3	1.53	0.73
1:A:266:LYS:HE3	1:A:266:LYS:HA	1.71	0.72
1:B:263:ARG:HB3	4:B:304:HOH:O	1.90	0.72
1:A:61:PRO:HG2	1:A:64:LEU:HD12	1.70	0.71
1:A:2:ASP:HB2	1:A:78:LYS:O	1.90	0.69
1:B:266:LYS:HB2	4:B:304:HOH:O	1.93	0.69
1:B:240:LYS:HG2	4:B:366:HOH:O	1.92	0.69
1:A:111:ARG:HH11	1:A:111:ARG:CG	2.06	0.69
1:B:62:PHE:O	1:B:65:VAL:HG23	1.92	0.68
1:B:213:GLN:HG2	4:B:400:HOH:O	1.94	0.68
1:A:195:ALA:HB1	1:A:200:LYS:HE2	1.76	0.68
1:A:62:PHE:O	1:A:65:VAL:HG23	1.94	0.68
1:A:3:ILE:HB	1:A:79:ALA:HB2	1.75	0.68
1:B:64:LEU:HD21	1:B:273:VAL:HG23	1.77	0.67
1:B:282:PRO:HB3	4:B:385:HOH:O	1.93	0.66
1:B:14:ARG:HD3	4:B:401:HOH:O	1.93	0.66
1:A:190:LYS:HE2	1:A:196:SER:H	1.61	0.65
1:A:81:ILE:N	1:A:81:ILE:HD12	2.12	0.65
1:A:195:ALA:O	1:A:196:SER:O	2.16	0.64
1:B:169:LEU:HD23	1:B:172:GLN:HG3	1.78	0.64
1:A:240:LYS:NZ	1:A:240:LYS:HB2	2.12	0.63
1:B:152:TYR:OH	1:B:227:GLY:HA3	1.98	0.63
1:A:112:ILE:HG22	1:A:113:GLU:N	2.12	0.63
1:A:190:LYS:NZ	1:A:196:SER:HA	2.14	0.63
1:B:110:LYS:HD2	1:B:110:LYS:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:THR:OG1	1:B:214:THR:HG22	2.00	0.62
1:A:165:PRO:HG2	1:A:169:LEU:CD1	2.30	0.61
1:A:89:GLU:HG2	1:A:129:ARG:HE	1.64	0.61
1:A:165:PRO:HG2	1:A:169:LEU:HD12	1.82	0.61
1:B:31:PHE:HB2	1:B:267:ALA:HB1	1.83	0.60
1:A:36:TYR:O	1:A:37:ARG:HB2	2.02	0.60
1:A:190:LYS:HB2	1:A:196:SER:N	2.14	0.60
1:A:197:LYS:C	1:A:199:ASP:H	2.04	0.60
1:B:169:LEU:HA	1:B:172:GLN:HB2	1.84	0.60
1:A:167:THR:HG23	1:A:194:GLY:H	1.65	0.59
1:A:89:GLU:HB2	1:A:127:VAL:HA	1.85	0.59
1:B:53:LEU:HD12	1:B:270:MET:HG2	1.85	0.59
1:A:69:LYS:HD2	1:A:72:CYS:SG	2.44	0.58
1:B:107:SER:OG	1:B:108:GLY:N	2.31	0.58
1:B:110:LYS:HB3	1:B:110:LYS:NZ	2.18	0.58
1:A:218:GLN:HG2	1:A:222:TRP:CD2	2.38	0.58
1:B:268:ASN:C	1:B:268:ASN:HD22	2.06	0.57
1:A:212:TRP:CE3	1:A:241:SER:HB3	2.39	0.57
1:A:89:GLU:HG2	1:A:129:ARG:NE	2.20	0.57
1:B:268:ASN:C	1:B:268:ASN:ND2	2.57	0.57
1:A:138:SER:C	1:A:140:GLY:H	2.08	0.57
1:A:201:TYR:CD2	1:A:201:TYR:N	2.71	0.56
1:A:69:LYS:HE3	4:A:386:HOH:O	2.06	0.56
1:A:124:GLU:HG3	1:A:280:PHE:CE1	2.40	0.56
1:A:36:TYR:O	1:A:37:ARG:CB	2.53	0.56
1:A:167:THR:CG2	1:A:194:GLY:H	2.19	0.56
1:A:17:CYS:SG	1:A:58:ARG:NH2	2.78	0.56
1:B:222:TRP:O	1:B:225:GLN:HG2	2.07	0.55
1:B:170:THR:HG22	1:B:190:LYS:HG2	1.89	0.55
1:B:212:TRP:O	1:B:216:VAL:HG23	2.06	0.55
1:A:30:SER:HB2	1:A:52:ARG:HD2	1.89	0.55
1:B:165:PRO:HG2	1:B:169:LEU:HD12	1.89	0.55
1:A:69:LYS:HA	1:A:72:CYS:SG	2.47	0.55
1:A:192:GLY:N	1:A:195:ALA:HB2	2.22	0.55
1:A:107:SER:HB2	1:A:112:ILE:HG13	1.89	0.54
1:A:138:SER:O	1:A:140:GLY:N	2.40	0.54
1:A:150:ARG:NH1	1:A:154:GLU:OE2	2.34	0.54
1:A:170:THR:HG22	1:A:190:LYS:HD2	1.89	0.54
1:B:107:SER:O	1:B:179:ASP:OD1	2.25	0.54
1:A:67:GLN:NE2	4:A:354:HOH:O	2.40	0.54
1:B:20:SER:O	1:B:24:GLU:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:HIS:O	1:B:263:ARG:HD3	2.07	0.54
1:B:17:CYS:SG	1:B:58:ARG:NH1	2.81	0.54
1:B:110:LYS:HD2	1:B:110:LYS:N	2.22	0.54
1:B:211:THR:O	1:B:215:VAL:HG23	2.08	0.53
1:B:170:THR:HG22	1:B:190:LYS:CG	2.39	0.53
1:A:124:GLU:HG3	1:A:280:PHE:CZ	2.44	0.53
1:A:190:LYS:O	1:A:200:LYS:HD3	2.09	0.53
1:A:197:LYS:C	1:A:199:ASP:N	2.62	0.53
1:B:130:ARG:NH1	4:B:395:HOH:O	2.42	0.53
1:B:26:ARG:HB3	1:B:52:ARG:HD3	1.91	0.52
1:B:89:GLU:HG2	1:B:129:ARG:HE	1.74	0.52
1:A:112:ILE:HG22	1:A:113:GLU:H	1.73	0.51
1:A:199:ASP:O	1:A:200:LYS:O	2.27	0.51
1:B:13:VAL:HG21	1:B:65:VAL:HG22	1.93	0.51
1:B:268:ASN:ND2	4:B:304:HOH:O	2.42	0.51
1:A:235:HIS:CD2	1:A:259:SER:OG	2.64	0.50
1:B:13:VAL:HG11	1:B:65:VAL:HG21	1.92	0.50
1:A:111:ARG:HB3	1:A:111:ARG:NH1	2.18	0.50
1:B:53:LEU:CD1	1:B:270:MET:HG2	2.40	0.50
1:A:220:LYS:HD3	4:A:418:HOH:O	2.12	0.50
1:A:102:LYS:HB3	4:A:344:HOH:O	2.11	0.50
1:A:222:TRP:O	1:A:225:GLN:HG2	2.12	0.50
1:A:133:LEU:HB3	1:A:135:LEU:HD11	1.92	0.49
1:A:190:LYS:HE2	1:A:196:SER:N	2.27	0.49
1:B:232:ASP:O	1:B:233:GLU:HB2	2.12	0.49
1:B:190:LYS:HE3	1:B:199:ASP:OD2	2.13	0.49
1:A:191:ILE:C	1:A:195:ALA:HB2	2.32	0.49
1:A:21:THR:HG21	4:A:303:HOH:O	2.11	0.49
1:B:124:GLU:HG3	1:B:280:PHE:CE1	2.48	0.49
1:A:219:PRO:HG2	1:A:222:TRP:HB2	1.96	0.48
1:A:99:TRP:O	1:A:102:LYS:HG3	2.13	0.48
1:B:7:PHE:CD1	1:B:84:GLN:HG2	2.49	0.47
1:B:26:ARG:HD3	4:B:389:HOH:O	2.14	0.47
1:B:165:PRO:HG2	1:B:169:LEU:CD1	2.43	0.47
1:B:220:LYS:HG2	4:B:330:HOH:O	2.14	0.47
1:B:14:ARG:HB3	1:B:59:LEU:HD23	1.97	0.47
1:A:232:ASP:O	1:A:233:GLU:HB2	2.15	0.47
1:B:211:THR:CB	1:B:213:GLN:HG3	2.44	0.47
1:A:201:TYR:N	1:A:201:TYR:HD2	2.13	0.47
1:A:161:LEU:O	1:A:229:MET:HA	2.15	0.47
1:A:53:LEU:HD12	1:A:270:MET:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLU:OE1	1:B:55:ASP:HB2	2.15	0.46
1:B:8:HIS:O	1:B:12:HIS:O	2.33	0.46
1:A:189:LYS:CE	1:A:200:LYS:HD2	2.45	0.46
1:A:6:HIS:HD2	4:A:348:HOH:O	1.98	0.46
1:A:111:ARG:HH11	1:A:111:ARG:HG2	1.81	0.46
1:A:111:ARG:CG	1:A:111:ARG:NH1	2.71	0.46
1:B:269:ILE:O	1:B:273:VAL:HG22	2.16	0.46
1:A:190:LYS:O	1:A:195:ALA:HB1	2.17	0.45
1:B:2:ASP:HB2	1:B:78:LYS:O	2.16	0.45
1:B:167:THR:HG23	1:B:194:GLY:CA	2.45	0.45
1:B:180:TYR:O	1:B:181:ARG:HB2	2.16	0.45
1:A:111:ARG:NH1	1:A:111:ARG:HG2	2.31	0.45
1:A:231:ASN:ND2	1:A:234:CYS:HA	2.32	0.45
1:A:9:ASP:HB2	1:A:250:ASN:O	2.17	0.45
1:A:37:ARG:HA	1:A:42:PHE:CE2	2.52	0.45
1:A:189:LYS:HE2	1:A:200:LYS:HD2	1.98	0.45
1:B:78:LYS:HA	1:B:78:LYS:HE2	1.99	0.45
1:A:193:GLY:C	1:A:195:ALA:H	2.20	0.44
1:B:167:THR:O	1:B:170:THR:HB	2.18	0.44
1:A:152:TYR:OH	1:A:227:GLY:HA3	2.17	0.44
1:B:167:THR:HG23	1:B:194:GLY:HA2	1.99	0.44
1:B:70:LYS:H	1:B:70:LYS:CD	2.31	0.44
1:A:263:ARG:NH1	4:A:411:HOH:O	2.51	0.44
1:A:3:ILE:HB	1:A:79:ALA:CB	2.43	0.43
1:B:94:LYS:CD	1:B:94:LYS:N	2.74	0.43
1:A:240:LYS:HB2	1:A:240:LYS:HZ3	1.83	0.43
1:A:195:ALA:C	1:A:196:SER:O	2.56	0.43
1:A:196:SER:CB	1:A:200:LYS:HG3	2.43	0.43
1:A:180:TYR:O	1:A:181:ARG:HB2	2.18	0.43
1:A:8:HIS:O	1:A:12:HIS:O	2.37	0.43
1:A:112:ILE:CG2	1:A:113:GLU:N	2.79	0.43
1:A:139:ALA:O	1:A:140:GLY:C	2.57	0.43
1:A:200:LYS:HB3	1:A:201:TYR:H	1.55	0.43
1:B:130:ARG:HA	1:B:255:LYS:O	2.19	0.43
1:B:141:ARG:HD3	1:B:258:LEU:HB3	2.00	0.43
1:B:153:LEU:HD11	1:B:187:MET:CE	2.49	0.43
1:A:196:SER:C	1:A:197:LYS:O	2.57	0.42
1:B:235:HIS:CD2	1:B:259:SER:OG	2.72	0.42
1:B:3:ILE:HD12	1:B:72:CYS:SG	2.59	0.42
1:B:67:GLN:NE2	4:B:387:HOH:O	2.45	0.42
1:A:249:LEU:HB3	1:A:252:CYS:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:LEU:CD2	1:B:273:VAL:HG23	2.45	0.42
1:A:19:GLU:OE2	1:A:19:GLU:HA	2.19	0.42
1:A:78:LYS:HA	1:A:78:LYS:CE	2.39	0.42
1:A:235:HIS:HD2	1:A:259:SER:OG	2.03	0.42
1:A:240:LYS:O	1:A:244:SER:HB2	2.20	0.41
1:A:240:LYS:HB2	1:A:240:LYS:HZ2	1.84	0.41
1:A:116:TRP:HB2	1:B:220:LYS:HZ2	1.85	0.41
1:B:185:HIS:HD2	4:B:319:HOH:O	2.03	0.41
1:B:197:LYS:HD3	1:B:197:LYS:HA	1.85	0.41
1:A:81:ILE:N	1:A:81:ILE:CD1	2.82	0.41
1:A:263:ARG:HB3	1:A:266:LYS:HB2	2.01	0.41
1:A:63:GLY:HA3	1:A:273:VAL:O	2.21	0.41
1:A:75:PHE:HB2	1:A:77:TYR:CD2	2.56	0.40
1:A:104:GLU:HA	1:A:111:ARG:NH2	2.37	0.40
1:B:81:ILE:N	1:B:81:ILE:HD12	2.36	0.40
1:A:147:LEU:HD23	1:A:147:LEU:HA	1.90	0.40
1:B:202:LYS:HB3	1:B:205:ALA:HB2	2.03	0.40
1:B:211:THR:OG1	1:B:213:GLN:CG	2.64	0.40
1:B:268:ASN:HD22	1:B:269:ILE:N	2.20	0.40
1:B:168:ALA:HB3	4:B:393:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	280/282 (99%)	259 (92%)	14 (5%)	7 (2%)	<b>5</b> <b>2</b>
1	B	280/282 (99%)	264 (94%)	12 (4%)	4 (1%)	<b>11</b> <b>5</b>
All	All	560/564 (99%)	523 (93%)	26 (5%)	11 (2%)	<b>7</b> <b>3</b>

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	ALA
1	A	196	SER
1	A	200	LYS
1	B	34	ASP
1	A	9	ASP
1	A	37	ARG
1	A	195	ALA
1	A	197	LYS
1	B	9	ASP
1	B	199	ASP
1	B	202	LYS

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	247/247 (100%)	230 (93%)	17 (7%)	15	11
1	B	247/247 (100%)	230 (93%)	17 (7%)	15	11
All	All	494/494 (100%)	460 (93%)	34 (7%)	15	11

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	52	ARG
1	A	54	LEU
1	A	102	LYS
1	A	111	ARG
1	A	131	ARG
1	A	135	LEU
1	A	150	ARG
1	A	153	LEU
1	A	161	LEU
1	A	199	ASP
1	A	201	TYR
1	A	218	GLN

*Continued on next page...*

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	220	LYS
1	A	266	LYS
1	A	268	ASN
1	A	278	GLU
1	B	21	THR
1	B	62	PHE
1	B	70	LYS
1	B	91	LEU
1	B	94	LYS
1	B	110	LYS
1	B	113	GLU
1	B	143	LEU
1	B	161	LEU
1	B	167	THR
1	B	190	LYS
1	B	213	GLN
1	B	221	GLU
1	B	253	MET
1	B	264	ASP
1	B	268	ASN
1	B	275	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	6	HIS
1	A	74	ASN
1	A	134	ASN
1	A	145	GLN
1	A	185	HIS
1	A	218	GLN
1	A	225	GLN
1	A	231	ASN
1	A	235	HIS
1	A	268	ASN
1	B	23	HIS
1	B	67	GLN
1	B	74	ASN
1	B	185	HIS
1	B	225	GLN
1	B	235	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.